Robust Summary – ACC Phthalate Esters Panel

Physical Chemical Elements
1) Melting Point

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
Remarks	
METHOD	
Method	Calculated by MBBPWIN ver. 1.40
GLP	N
Year	2000
Remarks	MP based on the average results of the calculation methods of K. Joback and Gold and Ogle.
RESULTS	
Value	152°C
Decomposition	N
Sublimation	N
Remarks	Calculated SAR result for surrogate structure contained in program database (smilecas.dat).
CONCLUSIONS	
DATA QUALITY	
Reliability	(2) Reliable with restrictions
Remarks	EPIWIN is used and advocated by the US EPA for chemical property estimation. This class of compounds is mainly liquids and have considerably lower melting points than predicted by the model.
REFERENCES	Meylan, M. SRC 1994-1999. MBBPWIN is contained in the computer program EPIWIN (Estimate ver. 3.04), available from Syracuse Research Corp.
Source	ExxonMobil Biomedical Sciences, Inc. Annadale, NJ.

Robust Summary – ACC Phthalate Esters Panel

Physical Chemical Elements
2) Boiling Point

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
Remarks	
METHOD	
Method	Calculated by MBBPWIN ver. 1.40
GLP	N
Year	2000
Remarks	BP based on the average results of the calculation methods of S. Stein and R. Brown..
RESULTS	
Value	474°C
Pressure	1.0
Pressure Unit	Atm
Decomposition	N
Remarks	Calculated SAR result for surrogate structure contained in program database (smilecas.dat).
CONCLUSIONS	
DATA QUALITY	
Reliability	(2) Reliable with restrictions
Remarks	EPIWIN is used and advocated by the US EPA for chemical property estimation.
REFERENCES	Meylan, M. SRC 1994-1999. MBBPWIN is contained in the computer program EPIWIN (Estimate ver. 3.04), available from Syracuse Research Corp.
Source	ExxonMobil Biomedical Sciences, Inc. Annadale, NJ.

Robust Summary – ACC Phthalate Esters Panel

Physical Chemical Elements
3) Vapor Presure

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
Remarks	
METHOD	
Method	Calculated by MBBPWIN ver. 1.40
GLP	N
Year	2000
Remarks	VP based on the modified calculation method of Grain.
RESULTS	
Value	8.48E-07 Pa
Temperature	25°C
Decomposition	N
Remarks	Calculated SAR result for surrogate structure contained in program database (smilecas.dat).
CONCLUSIONS	
DATA QUALITY	
Reliability	(2) Reliable with restrictions
Remarks	EPIWIN is used and advocated by the US EPA for chemical property estimation.
REFERENCES	Meylan, M. SRC 1994-1999. MBBPWIN is contained in the computer program EPIWIN (Estimate ver. 3.04), available from Syracuse Research Corp.
Source	ExxonMobil Biomedical Sciences, Inc. Annadale, NJ.

Robust Summary – ACC Phthalate Esters Panel

Physical Chemical Elements
4) Partition Coefficient

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
Remarks	
METHOD	
Method	Calculated by LOGKOWWIN ver. 1.65
GLP	N
Year	2000
Remarks	BP based on the atom/fragment contribution method of W. Meylan and P. Howard.
RESULTS	
Log Pow	7.0
Temperature	25°C
Remarks	Calculated SAR result for surrogate structure contained in program database (smilecas.dat).
CONCLUSIONS	
DATA QUALITY	
Reliability	(2) Reliable with restrictions
Remarks	EPIWIN is used and advocated by the US EPA for chemical property estimation.
REFERENCES	Meylan, M. SRC 1994-1999. MBBPWIN is contained in the computer program EPIWIN (Estimate ver. 3.04), available from Syracuse Research Corp.
Source	ExxonMobil Biomedical Sciences, Inc. Annadale, NJ.

Robust Summary – ACC Phthalate Esters Panel

Physical Chemical Elements
5) Water Solubility

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
Remarks	
METHOD	
Method	Calculated by WSKOWWIN ver. 1.3.6.
GLP	N
Year	2000
Remarks	Calculation based on a Kow correlation method of M. Meylan and P. Howard.
RESULTS	
Value at temperature	0.00147 mg/L at 25°C
Description of solubility	N
pH value	
pKa value	
Remarks	Calculated SAR result for surrogate structure contained in program database (smilecas.dat).
CONCLUSIONS	
DATA QUALITY	
Reliability	(2) Reliable with restrictions
Remarks	EPIWIN is used and advocated by the US EPA for chemical property estimation.
REFERENCES	Meylan, M. SRC 1994-1999. MBBPWIN is contained in the computer program EPIWIN (Estimate ver. 3.04), available from Syracuse Research Corp.
Source	ExxonMobil Biomedical Sciences, Inc. Annadale, NJ.

Robust Summary – ACC Phthalate Esters Panel

Physical Chemical Elements
6) Photodegradation

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
Remarks	
METHOD	
Method	Calculated by APOWIN ver. 1.89.
Test (test type)	Calculation
GLP	N
Year	2000
Light source	Sunlight
Light spectrum	Natural sunlight
Relative intensity	1
Spectrum of substance	
Remarks	Method based on the work of Atkinson.
RESULTS	
Conc. of substance	
Temperature	25°C
Direct photolysis	
Half-life	
Degradation %	
Quantum yield	
Indirect photolysis	Y
Sensitizer	OH radical
Conc. of sensitizer	1.50E+06 or radicals /cm^3
Rate constant	17.267 E-12 cm^3/molecule-sec
Half-life	0.619 d. (12 hour day)
Breakdown products	Unknown
Remarks	Calculated SAR result for surrogate structure contained in program database (smilecas.dat).
CONCLUSIONS	
DATA QUALITY	
Reliability	(2) Reliable with restrictions
Remarks	EPIWIN is used and advocated by the US EPA for chemical property estimation.
REFERENCES	Meylan, M. SRC 1994-1999. MBBPWIN is contained in the computer program EPIWIN (Estimate ver. 3.04), available from Syracuse Research Corp.
Source	ExxonMobil Biomedical Sciences, Inc. Annadale, NJ.

Robust Summary – ACC Phthalate Esters Panel

Physical Chemical Elements
7) Stability in water (hydrolysis)

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
Remarks	
METHOD	
Method	Calculated by HYDROWIN ver.1.67.
Type (test)	Calculation
GLP	N
Year	2000
Remarks (conditions, analysis, duration, controls)	Calculation of Kb1 at pH 7 and 25°C, specific base catalyzed hydrolysis. Calculation based on work by T. Mill et al. SRI under EPA contract. Calculated SAR result for surrogate structure contained in program database (smilecas.dat).
RESULTS	
Measured value	
Degradation %	
Half-life	1.555 yr
Breakdown products	Hydrolysis is to monoester and free alcohol
CONCLUSIONS	
DATA QUALITY	
Reliability	(2) Reliable with restrictions
Remarks	EPIWIN is used and advocated by the US EPA for chemical property estimation.
REFERENCES	Meylan, M. SRC 1994-1999. MBBPWIN is contained in the computer program EPIWIN (Estimate ver. 3.04), available from Syracuse Research Corp.
Source	ExxonMobil Biomedical Sciences, Inc. Annadale, NJ.

Robust Summary – ACC Phthalate Esters Panel

Physical Chemical Elements
8) Transport/distribution (fugacity)

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
Remarks	
METHOD	
Test (test type)	Calculated according to Mackay Level 1
Method (Y/N)	Y
GLP	N
Year	2000
Remarks	Model based on fugacity. Physical properties input are those calculated by the EPIWIN Estimation 3.04 program and included in this summary.
RESULTS	
Media	Soil, air, water, suspended sediment and sediment
Distribution	Medium: % distribution Soil: 97.7 Air: 5.84E-04 Water: 0.011 Sus. Sediment: 0.068 Sediment: 2.172
Remarks	Mobility in the environment is low due to low water solubility and low vapor pressure; chemical will adhere to soil/sediment and not be rapidly transported.
CONCLUSIONS	
DATA QUALITY	
Reliability	(2) Reliable with restrictions
Remarks	EPIWIN is used and advocated by the US EPA for chemical property estimation.
REFERENCES	Mackay, D., DiGuardo, A., Paterson, S., and C. Cowan. EQC Model ver. 1.01, 1997 available from the Environmental Modeling Centre, Trent University, Canada
Source	ExxonMobil Biomedical Sciences, Inc. Annadale, NJ.

Robust Summary – ACC Phthalate Esters Panel

Algal toxicity

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
Remarks	
METHOD	
Method/guideline	US EPA Algal Assay Procedure: Bottle Test. 1971 National Eutrophication Research Program, Pacific Northwest Water Laboratory
Type (test type)	Static acute
GLP	N
Year	1979
Species	Selanstrum capricornutum
Analytical monitoring	N
Exposure period	24, 48, 72 and 96 hours
Statistical methods	N
Test conditions	Triplicate algal cultures were incubated at 24 ±1°C under approx 4000 lux illumination. Test exposure levels were based on pilot testing; nominal test concentrations were 0, 360, 600 and 1000 mg/L. pH was 7.2 at study initiation and 7.2 to 7.4 at 96 hours. Cell number and chlorophyll content were measured at 24, 48, 72 and 96 hours.
RESULTS	
Concentration	Did not measure
Units	Mg/L nominal
Value	Based on cell number and decrease in *in vivo* chlorophyll content, EC50 at each time point was >1000mg/L.
Conclusion	
CONCLUSIONS	
DATA QUALITY	
Reliability	(2) Reliable with restrictions
Remarks	
REFERENCES	Toxicity of S-278 to the freshwater algae Selanstrum capricornutum. EG&G Bionomics Marine Research , Pensacola, Florida, April, 1979.
Source	Toxicology Consultants, Inc., Gibsonia, PA. October, 2005

Robust Summary – ACC Phthalate Esters Panel

Fish toxicity

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
METHOD	
Method/guideline	Standard Methods for Examination of Water and Wastewater and Methods of Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians
Type (test type)	Static Acute
GLP	No, but study conduct and reporting was subject to laboratory Quality Assurance inspections, audits and reviews
Year	1979
Species	Pimephales promelas
Analytical monitoring	No
Exposure period	24, 48 and 96 hours
Statistical methods	Probit Analysis
Test conditions	10 fish per vessels were employed in 5 gallon glass aquaria containing 15 liters of water. Water parameters were; DO = 8.8mg/L; pH = 7.8. total hardness = 240 mg/L $CaCO_3$, total alkalinity = 360 mg/L $CaCO_3$ Testing temperature was 22°C. Fish were acclimated and held without food for 48hours prior to testing. Exposure was to a single dose level of 1000mg test material /L. A positive control, antimycin A, was used. Because DO levels dropped to about 50% saturation, aeration of test aquaria was used.
RESULTS	
Concentration	Nominal test concentration = 1000mg/L
Units	Mg/L
Value	96-hour LC50 > 1000mg/L
Conclusion	No significant toxicity observed at or below the test substance water solubility.
DATA QUALITY	
Reliability	(2) Reliable with restrictions
REFERENCES	Acute Toxicity of S-278 to the Fathead Minnows. ABC Laboratories, Columbia, MO., 1979 Committee on Methods for Toxicity Tests with Aquatic Organisms, C. E. Stephan, 1975, Methods of Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA Ecological research Series EPA-660/3-75-009, April, 1975.
Source	Toxicology Consultants, Inc., Gibsonia, PA. October, 2005

Robust Summary – ACC Phthalate Esters Panel

Fish toxicity

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
METHOD	
Method/guideline	Standard Methods for Examination of Water and Wastewater and Methods of Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians
Type (test type)	Static Acute
GLP	No, but study conduct and reporting was subject to laboratory Quality Assurance inspections, audits and reviews
Year	1979
Species	Salmo gairdneri
Analytical monitoring	No
Exposure period	24, 48 and 96 hours
Statistical methods	Probit Analysis
Test conditions	10 fish per vessels were employed in 5 gallon glass aquaria containing 15 liters of water. Water parameters were; DO = 8.9mg/L; pH = 7.8. total hardness = 240 mg/L $CaCO_3$, total alkalinity = 360 mg/L $CaCO_3$ Testing temperature was 22°C. Fish were acclimated and held without food for 48hours prior to testing. Exposure was to a single dose level of 1000mg test material /L. A positive control, antimycin A, was used.
RESULTS	
Concentration	Nominal test concentration = 1000mg/L
Units	Mg/L
Value	96-hour LC50 > 1000mg/L
Conclusion	No significant toxicity observed at or below the test substance water solubility.
DATA QUALITY	
Reliability	(2) Reliable with restrictions
REFERENCES	Acute Toxicity of S-278 to the Rainbow Trout. ABC Laboratories, Columbia, MO., 1979 Committee on Methods for Toxicity Tests with Aquatic Organisms, C. E. Stephan, 1975, Methods of Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA Ecological research Series EPA-660/3-75-009, April, 1975.
Source	Toxicology Consultants, Inc., Gibsonia, PA. October, 2005

Robust Summary – ACC Phthalate Esters Panel

Daphnia toxicity

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
METHOD	
Method/guideline	Methods of Acute Toxicity Tests with Aquatic Organisms
Type (test type)	Static Acute
GLP	No but study conduct and reporting was subject to laboratory Quality Assurance inspections, audits and reviews
Year	1979
Species	Daphnia magna
Analytical monitoring	No
Exposure period	24 and 48 hours
Statistical methods	Probit Analysis
Test conditions	Adults Daphnids, 20 per vessels, were employed in 250 mlglass aquaria containing 200 mls of water. Water parameters were; DO = 9.2mg/L; pH = 7.9. Testing temperature was 20°C. Exposure was to a single dose level of 1.0, 1.8, 3.2, 5.6, and 10mg test material /L. A negative and an acetone control were used. Test material was formulated in acetone.
RESULTS	
Mortality	0/20, 0/20, 0/20, 3/20, 17/20 @ 1.0, 1.8, 3.2, 5.6 and 10 mg/L
Units	Mg/L (nominal)
Value	48 hour EC50 = 7.5mg/L (6.6 – 8.5 CI)
Conclusion	Mortalities observed at test material concentrations exceeding water solubility. It is likely that Daphnia mortality was due to physical entrapment of the insoluble test material rather than chemical toxicity.
DATA QUALITY	
Reliability	(2) Reliable with restrictions
REFERENCES	Acute Toxicity of S-278 to the Daphnia magna. ABC Laboratories, Columbia, MO., 1979 Committee on Methods for Toxicity Tests with Aquatic Organisms, C. E. Stephan, 1975, Methods of Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA Ecological research Series EPA-660/3-75-009, April, 1975.
Source	Toxicology Consultants, Inc., Gibsonia, PA. October, 2005

Robust Summary – ACC Phthalate Esters Panel

Mammalian toxicity

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
METHOD	
Method/guideline	Not stated.
Type (test type)	Acute oral gavage
GLP	No
Year	1969
Species	Rat Sprague-Dawley male and female
Analytical monitoring	No
Exposure period	Single dosing followed by 9 day observation period
Statistical methods	None
Test conditions	One male or female rat per dose received a single oral gavage dose of 2,000 to 15,800 mg/kg.; Toxic signs and weight gain were monitored; all animals were necropsied.
RESULTS	
Mortality	Al animals survived to necropsy
Units	Mg/kg
Value	Acute oral LD50 > 18,500 mg/kg
Conclusion	Test material is practically acutely nontoxic orally
DATA QUALITY	
Reliability	(2) Reliable with restrictions
REFERENCES	Younger Laboratories, St. Louis, MO., Toxicological Investigations of Santicizer 278, 1969.
Source	Toxicology Consultants, Inc., Gibsonia, PA. October, 2005

Robust Summary – ACC Phthalate Esters Panel

Mammalian toxicity

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
METHOD	
Method/guideline	Not stated.
Type (test type)	Skin absorption
GLP	No
Year	1969
Species	Rabbit, New Zealand male and female
Analytical monitoring	No
Exposure period	Single exposure followed by 14 day observation period
Statistical methods	None
Test conditions	One male or female rabbit per dose received a single dermal application of 2510 to 10000mg/kg test material to clipped, intact skin. The application site was covered with plastic strips for 24 hours and the animals were held for 14 days post dosing. Toxic signs and weight gain were monitored; all animals were necropsied.
RESULTS	
Mortality	Al animals survived to necropsy
Units	Mg/kg
Value	Acute dermal LD50 > 10,000 mg/kg
Conclusion	Test material is practically acutely nontoxic dermally
DATA QUALITY	
Reliability	(2) Reliable with restrictions
REFERENCES	Younger Laboratories, St. Louis, MO., Toxicological Investigations of Santicizer 278, 1969.
Source	Toxicology Consultants, Inc., Gibsonia, PA. October, 2005

Robust Summary – ACC Phthalate Esters Panel

Mammalian toxicity

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
METHOD	
Method/guideline	Not stated. Dermal reaction scoring according to the method of Draize.
Type (test type)	Skin irritation
GLP	No
Year	1969
Species	Rabbit, New Zealand male and female
Analytical monitoring	No
Exposure period	Single 24-hour exposure followed by 7 day observation period
Statistical methods	None
Test conditions	Three male or female rabbits received a single dermal application of undiluted test material to clipped, intact skin. Amount applied not stated. The application site was covered with plastic strips for 24 hours and the animals were held for 7 days post dosing.
RESULTS	
Dermal Reaction	Eryhema and edema scores not given; average maximum irritation score occurred at 24 hours post application and was 0.6 out of a possible 8.0
Conclusion	Test material is considered nonirritating to the intact skin.
DATA QUALITY	
Reliability	(2) Reliable with restrictions
REFERENCES	Younger Laboratories, St. Louis, MO., Toxicological Investigations of Santicizer 278, 1969. Draize, J. H., J. of Pharm ad Exp. Therapeutics, Vol 38, December, 1944.
Source	Toxicology Consultants, Inc., Gibsonia, PA. October, 2005

Robust Summary – ACC Phthalate Esters Panel

Mammalian toxicity

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
METHOD	
Method/guideline	Not stated. Ocular reaction scoring according to the method of Draize.
Type (test type)	Eye irritation
GLP	No
Year	1969
Species	Rabbit, New Zealand male and female
Analytical monitoring	No
Exposure period	0.1 ml instilled into conjunctival sac. Exposure followed by 7 day observation period
Statistical methods	None
Test conditions	Three male or female rabbits received a single instillation of undiluted test material into their conjunctival sac. 24 post application the eyes were rinsed with warm isotonic saline. Animals were held for 7 days post dosing.
RESULTS	
Ocular Reaction	Eryhema and edema scores not given; average maximum irritation score occurred at 1 hour post application and was 4.0 out of a possible 110.0
Conclusion	Test material is considered slightly irritating to the eye.
DATA QUALITY	
Reliability	(2) Reliable with restrictions
REFERENCES	Younger Laboratories, St. Louis, MO., Toxicological Investigations of Santicizer 278, 1969. Draize, J. H., J. of Pharm ad Exp. Therapeutics, Vol 38, December, 1944.
Source	Toxicology Consultants, Inc., Gibsonia, PA. October, 2005

Robust Summary – ACC Phthalate Esters Panel

Genetic toxicity

TEST SUBSTANCE	
Identity	Phthalic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate
CAS #	16883-83-3
METHOD	
Method/guideline	Ames/Salmonella plate incorporation
Type (test type)	Bacterial point mutation
GLP	No
Year	1982
Strains	Salmonella typhimurium TA 98, TA100, TA1535, TA1537, TA 1538
Analytical monitoring	No
Statistical methods	Bartlett's test for homogeneity of variance, one sided t-test, Grubb's test for outlier data points, dose-response analyzed by regression analysis, overall significance by t-test.
Test conditions	Plate incorporation with and without rat liver postmitochondrial microsome preparation, Livers were Aroclor-induced. Cytotoxicity and solubility pilot studies were performed prior to the definitive study. A maximum of 10 µl test material was added to culture plates.
RESULTS	
Mutation activity	The number of revertant colonies induced by treatment with the test material in the presence and absence of exogenous metabolic activation was not significantly raised above background levels.
Conclusion	The test material was not mutagenic in this test system.
Comment	Levels of 10 µl per plate were not cytotoxic with or without metabolic activation but levels of 3 µl per plate exceeded the solubility of the test material.
DATA QUALITY	
Reliability	(1) Reliable
REFERENCES	Monsanto Environmental Health Labortory, Ames/Salmonella Mutagenicity Assay of Santicizer 278. St. Louis, 1982. Unpublished Report.
Source	Toxicology Consultants, Inc., Gibsonia, PA. October, 2005

201-16122

I U C L I D

Data Set

Existing Chemical	:	
CAS No.	:	16883-83-3
EINECS Name	:	
EINECS No.	:	
TSCA Name	:	
Molecular Weight	:	
Molecular Formula	:	

Producer Related Part

Company	:	Ferro Corporation
Creation date	:	24-10-05

Substance Related Part

Company	:	Ferro Corporation
Creation date	:	24-10-05
Memo	:	ACC Phthalate Ester Panel HPV Testing Group - high MW phthalates
Printing date	:	
Revision date	:	
Date of last Update	:	
Number of Pages	:	10
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 OECD AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Partner	:	Dr. Marian Stanley
Date	:	
Street	:	1300 Wilson Blvd.
Town	:	22209 Arlington, VA
Country	:	United States
Phone	:	(703) 741-5623
Telefax	:	(703) 741-6091
Telex	:	
Cedex	:	
Remark	:	The American Chemistry Council Phthalate Esters Panel includes the following member companies: BASF Corporation CONDEA Vista Company Eastman Chemical Company ExxonMobil Chemical Company Ferro Corporation ICI Americas / Uniqema Sunoco Chemicals Teknor Apex Company

1.1 GENERAL SUBSTANCE INFORMATION

Substance type	:	organic
Physical status	:	liquid
Purity	:	% w/w

1.1.0 DETAILS ON TEMPLATE

Comment		This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following eleven CAS numbers: 68648-93-1 117-84-0 68515-40-2 68515-45-7 68515-43-5 84-77-5 3648-20-2 85507-79-5 111381-91-0 68515-4 16883-83-3
Remark		The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters. Phthalate esters are generally clear to yellow, oily liquids with high boiling

ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were further subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure. Eleven of the U.S. HPV chemicals fall into this subcategory, which include varying mixed isomers of linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl and ditridecyl phthalate. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

02.11.2001

1.7 USE PATTERN

Type	:	industrial
Category	:	Polymers industry
Remark	:	High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

2.1 MELTING POINT

Value	:	152 ° C
Decomposition	:	No
Sublimation	:	No
Method	:	Melting point calculation by MPBPWIN ver. 1.40 using calculation methods of Joback and Gold and Ogle
Year	:	2000
GLP	:	No
Test substance	:	
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation Melting point calculation seems to give erroneously high results for the phthalate esters
Source	:	
Reliability	:	

(5)

Value	:	
Sublimation	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	
Method	:	
Remark	:	
Source	:	
Reliability	:	

08.10.2001

(4)

2.2 BOILING POINT

Value	:	474 ° C
Decomposition	:	No
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Boiling point calculation by MPBPWIN ver. 1.40 using calculation method of Stein and Brown.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

08.10.2001

(4)

Value	:	
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	
Source	:	
Reliability	:	

08.10.2001

(2)

2.4 VAPOUR PRESSURE

Value	:	8.48E-7 PA at 25° C
Decomposition	:	No
Method		other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Decomposition	:	No
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.40 using calculation method of Grain.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

08.10.2001 (4)

Value		
Decomposition		
Method		
Year		
GLP		
Test substance		
Decomposition		
Remark		
Source		
Reliability		

2.5 PARTITION COEFFICIENT

Log pow	:	7.0 at 25° C
Method		other (calculated)
Year	:	2000
GLP	:	No
Test substance	:	
Remark	:	Partition coefficient by LOGKOWWIN ver. 1.65 using an atom/fragment calculation method of Meylan and Howard.
Source	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Reliability	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA

12.11.2001

Log pow	:	
Method		
Year	:	
GLP	:	
Test substance	:	
Method	:	
Remark	:	
Source	:	
Reliability	:	

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2.6.1 WATER SOLUBILITY

Value	:	.00147 other: mg/l at 25 ° C
Qualitative	:	
Pka	:	at 25 ° C
PH	:	at and ° C
Method	:	other
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Water solubility calculated using WSKOWIN ver 1.36 based on Kow correlation method of Meylan and Howard
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions
08.10.2001		(4)

Value	:	
Qualitative	:	
Pka	:	
PH	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	
Remark	:	
Source	:	
Reliability	:	
19.12.2000		(1)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spect.	:	nm
Rel. intensity	:	1 based on Intensity of Sunlight
Conc. of subst.	:	at 25 degree C
Indirect photolysis		
Sensitizer	:	OH
Conc. of sens.	:	1500000 molecule/cm3
Rate constant	:	17.267 E-12 cm3/(molecule*sec)
Degradation	:	% after
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.89 based on the methods of Atkinson.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (4)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at degree C
t1/2 pH7	:	1.555 year at 25 degree C
t1/2 pH9	:	at degree C
Deg. Product	:	not measured
Method	:	other (calculated)
Year	:	2000
GLP	:	
Test substance	:	
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPIWIN is used and advocated by the US EPA for chemical property estimation
Source	:	ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability	:	(2) valid with restrictions

19.12.2000 (4)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level I
Media	:	Other
Air (level I)	:	0
Water (level I)	:	0
Soil (level I)	:	97.7
Biota (level II / III)	:	
Soil (level II / III)	:	
Method	:	Other
Year	:	2000

Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
08.10.2001 (3)

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 2000
Result : Soil - 97.7%
Air – 5.84 E-4%
Water - 0.011%
Sediment - 2.17%
Suspended sed. - 0.068%
Source : ExxonMobil Biomedical Sciences, Inc. Annandale, N.J. USA
Reliability : (2) valid with restrictions
12.11.2001 (3)

(1) Cousins, I. and D. Mackay (2000), Correlating The Physical-Chemical Properties of Phthalate Eesters Using the 'three Solubility' approach, chemosphere 41:1389-1399.

(2) David, R., R. Mckee, J. Butala, R. Barter and M. Kayser, Chapter 81 - Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalchols, Patty's Industrial Hygiene and Toxicology, Fifth Edition, Volume 6, pp635-932, John Wiley & Sons, Inc., New York

(3) Mackay, D., A. DiGuardo, S. Paterson and C. Cowan, EQC Model ver. 1.01, 1997, available form the Emvironmental Centre, Trent Univ. Canada.

(4) Meylan, M. Syracuse Research Corporation (1994-1999) Calculation program contained in EPIWIN (Esitmate ver. 3.04) available from SRC.

(5) Staples, C., D. Peterson, T. Parkerton and W. Adams (1997), the Environmental Fate of Phthalate Esters: A literature Review, Chemosphere 35:667-749.

7.1 END POINT SUMMARY

7.2 HAZARD SUMMARY

Chapter : Chapters 2,3,4 & 5

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

02.11.2001

7.3 RISK ASSESSMENT